APPLIED ORGANOMETALLIC CHEMISTRY
Appl. Organometal. Chem. 2004; **18**: 197–198
Published online in Wiley InterScience (www.interscience.wiley.com). DOI:10.1002/aoc.596

Crystallographic report

(2,2′-Bipyridine)bis(*N*,*N*-dibenzyldithiocarbamato) zinc(II)

Chian Sing Lai and Edward R. T. Tiekink*

Department of Chemistry, National University of Singapore, Singapore 117543, Singapore

Received 13 December 2003; Revised 15 December 2003; Accepted 16 December 2003

The structure of $Zn[S_2CN(CH_2Ph)_2]_2$(2,2′-bipy) features a distorted trigonal prismatic geometry around the zinc centre defined by an N_2S_4 donor set; the molecule has two-fold symmetry. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; zinc; dithiocarbamate; diimine adduct

COMMENT

The aggregated structures of the binary zinc-triad 1,1-dithiolates[1] are disrupted by the addition of base to form, usually, monomeric species. The addition of 2,2′-bipyridine to the monomeric structure of $Zn[S_2CN(CH_2Ph)_2]_2$[2] leads to a distorted trigonal prismatic coordination geometry for zinc defined by an N_2S_4 donor set (Fig. 1), as the dithiocarbamate ligands are symmetrically chelating; the molecule has crystallographically imposed two-fold symmetry. The twist away from the ideal angle of 0° for a trigonal prismatic geometry is approximately 7°. Owing to variations in the mode of coordination of the dithiocarbamate ligands and the steric demands of the diimine ligands operating in these adducts, coordination geometries range from tetrahedral, e.g. $Zn[S_2CN(CH_2)_4]_2$(2,9-Me_2-1,10-phen),[3] to the more common distorted octahedral geometry.[4–6]

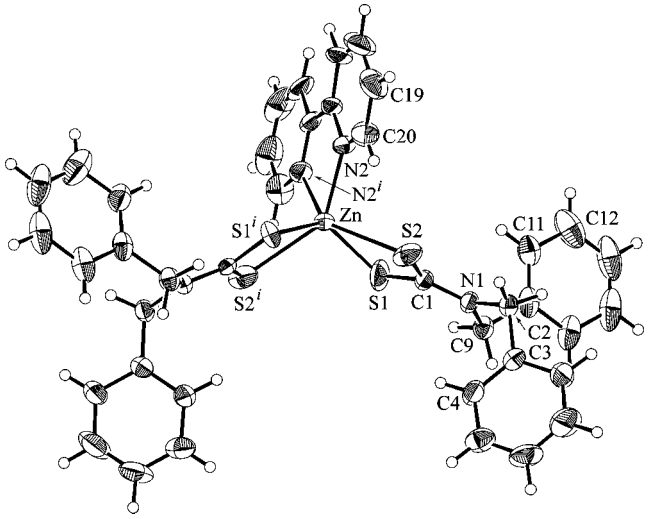

Figure 1. Molecular structure of $Zn[S_2CN(CH_2Ph)_2]_2$(2,2′-bipy). Key geometric parameters: Zn–S1 2.591(2), Zn–S2 2.586(2), Zn–N2 2.160(4), S1–C1 1.688(5), S2–C1 1.721(6), N1–C1 1.320(5) Å; S1–Zn–S2 68.10(5), S1–Zn–S1^i 139.44(10), S1–Zn–S2^i 92.93(6), S2–Zn–S2^i 124.66(9), N2–Zn–N2^i 74.6(3)°. Symmetry code *i*: $1-x, -y, z$.

EXPERIMENTAL

Yellow crystals of $Zn[S_2CN(CH_2Ph)_2]_2$(2,2′-bipy) were obtained from the slow evaporation of a chloroform solution containing equimolar amounts of $Zn[S_2CN(CH_2Ph)_2]_2$[2] and 2, 2′-bipyridine (Aldrich); m.p. 495–496 °C. IR (KBr): ν(C–S) 984 and ν(C–N) 1493 cm^{-1}. Data were collected at 223(2) K on a Bruker AXS SMART CCD for a plate of dimensions $0.05 \times 0.33 \times 0.49$ mm^3. $C_{40}H_{36}N_4S_4Zn$, $M = 766.37$, orthorhombic, *Pba*2, $a = 31.197(5)$, $b = 7.0247(11)$, $c = 8.4629(13)$ Å, $V = 1854.6(5)$ $Å^3$, $Z = 2$, 4419 unique data (θ_{max} 30.0°), 3049 data with $I \geq 2\sigma(I)$, $R = 0.064$ (obs. data), $wR = 0.171$ (all data). The structure was refined as a racemic twin using the TWIN and BASF commands in SHELXL-97. Programs used: teXsan, DIRDIF, SHELXL-97 and ORTEP. CCDC deposition number: 226725.

*Correspondence to: Edward R. T. Tiekink, Department of Chemistry, National University of Singapore, Singapore 117543, Singapore.
E-mail: chmtert@nus.edu.sg
Contract/grant sponsor: National University of Singapore; Contract/grant number: R-143-000-213-112.

Acknowledgements

The National University of Singapore (R-143-000-213-112) is thanked for support.

REFERENCES

1. Tiekink ERT. *CrystEngComm.* 2003; **5**: 101.
2. Decken A, Gossage RA, Chan MY, Lai CS, Tiekink ERT. *Appl. Organometal. Chem.* 2004; **18**: 101.
3. Lai CS, Tiekink ERT. *Appl. Organometal. Chem.* 2003; **17**: 255.
4. Tiekink ERT. *Z. Kristallogr. New Cryst. Struct.* 2001; **216**: 575 and references cited therein.
5. Qian J, Tiekink ERT. *Main Group Met. Chem.* 2002; **25**: 317.
6. Lai CS, Tiekink ERT. *Appl. Organometal. Chem.* 2003; **17**: 197.